

On Some Factors Affecting the Critical Temperature in a Two-Band Model of Superconductivity

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Abstract The influence of a few factors on the critical temperature in a two-band superconducting system is investigated. The system contains conventional Cooper pairs from a wider band (the d-band) as well as local pairs (local bipolarons) from a narrower band (the f-band), which are induced via a pair-exchange potential. These factors are the Coulomb repulsion between f-electrons, the position of the f-band with respect to the bottom of the d-band and two kinds of hopping in the f-band: a single-polaron hopping and a pair hopping. The Coulomb potential turns out to lower the critical temperature from higher values to the pure BCS one. Each of the kinds of hopping is treated by making use of perturbation theory. Pair hopping is incorporated as the first order correction but the hopping of single polarons enters as the second order one. Each of them increases this temperature on its own, however, the hopping of single polarons makes it stronger. The position of the f-band that corresponds to the site energy of a f-electron poses a very interesting case. There appear two peaks at two values of that energy meaning a rapid increase of the critical temperature due to the strong effect of the presence of local electron pairs. In this case one has to do with a purely chemical mechanism of the increase of the critical temperature.

Keywords Superconductivity · Two-band model · Fermion pairs · Critical temperature

1 Introduction

For last decades there has been much progress in the discovery of new phenomena in solid state physics. The high-temperature superconductivity or the so-called heavy-fermion superconductivity belongs to this class. An especially intriguing question became the problem of mechanisms leading to such effects. The crucial question is how the critical temperature can be increased in relation to the BCS values. The simplest way was to reconsider the expression for the critical temperature in the BCS theory and take into account the manipulation on the width of the narrow shell around the Fermi level on which the BCS interaction is defined to be nonzero and the magnitude of the coupling constant. However, in view of experimental facts such an approach seems at least insufficient. The internal structure of new superconducting materials is much more complicated than the structure of simple metals or their alloys. The conventional BCS theory based on the concept of the phonon-mediated two-electron attraction does not include this at all. That is why there have been invoked many proposals of mechanisms explaining not only higher critical temperatures but a lot of other features of new materials. For example new boson fields were suggested to mediate between electrons due to the weakness of the isotope effect in these exotic superconductors. Let us mention plasmons [1, 2], spin fluctuations [3, 4] or even excitons [5, 6]. Especially important is the fact that the critical temperature of cuprates strongly depends on doping and the crystal structure. Moreover, the significance of correlations between electrons is stressed by many authors [7, 8]. All of this entails the so called non-Fermi liquid behavior of the normal phase and the fact that some undoped high-temperature superconductors are Mott insulators with antiferromagnetically ordered ground state. Especially interesting is the fact that sufficient

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doping brings about the mixed valence of copper in cuprates what leads to the appearance of mobile holes or electrons. Moreover, it is widely known that the critical temperature is sensitive to the number of CuO_2 planes. Still there is no agreement if phonons are important concerning superconductivity in new materials. However, despite the very poor isotope effect in many high-temperature superconductors phonons are still regarded by some researchers to play an essential role [9, 10]. For example, a mixed mechanism of superconductivity in the new materials was considered. This concept joined the strong coupling between phonons and electrons with the spin fluctuations idea [11].

Multi-band models are usually invoked to describe superconductivity in new materials. One can mention here the d–p model [12], the three-state Hubbard model [13] or the boson–fermion model [10, 14–17]. In all of these models electric charge is transferred from one band to the other, however, in the latter case this exchanged charge is in the form of electron pairs (quasibosons). In this paper a two-band electron system is investigated. The critical temperature and different factors influencing this temperature are the main points of examining. One of the bands is assumed to be wider than the other one. Moreover, it is conjectured that the effective Coulomb interaction in the wider band (the d-band) is attractive and is dealt with the BCS approximation. In the narrower band (the f-band) the effective Coulomb potential is repulsive. In general, it is admitted that the charge can be exchanged both via a single-particle hybridization and a pair exchange potential. To deal with a simplified version of a Hamiltonian some terms in the Hamiltonian, for instance the single-particle hybridization, are neglected. In this case such a simplified Hamiltonian is equivalent to that one obtained and investigated by Micnas et al. in [10, 14], by Pawłowski and Robaszkiewicz in [15] and moreover Czart and Robaszkiewicz in [16, 17]. In those papers the boson–fermion model was derived from the periodic Anderson model by making use of the Lang–Firsov and the generalized Schrieffer–Wolf transformations and investigated by means of the mean field method. The ground state properties, thermodynamics and electrodynamics were profoundly examined. Their motive was to study some materials exhibiting the mixed valence, it is, such substances which contain ions of the same element differing by $2e$ concerning their valence. There is a multitude of them, for example, Ti_4O_7 , $\text{Na}_x\text{V}_2\text{O}_5$ or CsSbCl_6 and TlF_2 , which are not superconductors, but their ground state is charged-ordered. Besides some superconductors such as A_{15} , C_{15} , V_3Si , Nb_3Ge and cuprates such as the tungsten bronzes and the doped bismuthates ($\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ and $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$) display the existence of local pairs because all of them are characterized by the poor conductivity and narrow bands being the result of the strong coupling between phonons and electrons [14, 16, 17]. In these materials comes to the appearance of

so called bipolarons, it is, tightly bound electron pairs due to strong coupling electrons with local lattice deformations [10, 14, 18]. In order to investigate this, the mean field approach is invoked. As a result, one obtains two separated subsystems corresponding to two bands. In each of the bands electron pairs are present but in the f-band one has to deal with the local pairs induced by the pair-exchange potential. In this paper we follow the approach used in [10, 14–17] and in fact we are interested in factors which can affect the critical temperature of such a system. For example, the effect of the single-particle hopping is compared to that of the pair hopping. Of course, both take place in the narrower band and are treated as perturbations. The concept of pair hopping has been used so far in a few papers [10, 14–20]. It is believed that a Hamiltonian consisting of the single-electron hopping and the pair hopping with negative coupling constant shares many common features with the negative Hubbard model [19]. Here the appearance of the pair hopping can be justified by the presence of the pair exchange potential mixing Cooper pairs from the wider band with those from the narrower one. The single-electron hopping in the narrower band was not taken into account in [15–17] in contrast to the Coulomb repulsion in this band which was taken exactly into account. This interaction turns out to be an obstacle to get higher critical temperatures, which is in agreement with our expectations and with results obtained in [16, 17]. In those papers this interaction was incorporated into considerations both as the attraction and the repulsion. In the attractive case the superconducting state is stable and the critical temperature increases with the increase of the strength of the attraction. The repulsive interaction lowers this temperature to the zero at some critical repulsion and the transition to the normal state in the presence of this interaction is of the first order. The next factor to be investigated is the site-energy of f-electrons that can be understood as the position of the f-level with respect to the bottom of the d-band. As we shall see, on changing this position there appear two peaks of higher critical temperature. The stronger coupling constant of the pair-exchange potential is the higher they are. They grow out from a level representing the pure BCS critical temperature. It is quite possible that if the coupling constants of the pairing potential in the d-band and of the pair exchange potential were larger than those used in the calculations then the BCS critical temperature would necessarily be higher and these peaks would be so high as to get sufficiently high critical temperatures. These two peaks are accompanied by the change of the average number of electrons per lattice site. If the chemical potential is fixed in the middle of the d-band the average number of d-electrons per lattice site remains equal to the unity; however, this is not the case concerning the number of f-electrons. Shifting the f-level from $-\infty$ to ∞ one obtains the decrease of the average number of f-electrons per

lattice site from 2 to 0, respectively. In [10, 14, 16] the critical temperature has only one maximum not two and tends to zero as the f-band is shifted to $-\infty$ or ∞ . This is so because the authors assumed that there was no superconductivity on its own in the wider band. Superconductivity is induced in both of the bands by the pair-exchange potential. If this potential is discarded then superconductivity will be turned off.

This paper is to ask the question what happens with the critical temperature of a two-band fermion system with narrow bands if there appear some additional effects. Moreover, one can look at the problem from a different point of view—what is going to happen with this temperature if beside the conventional BCS channel there appears a new mechanism of superconductivity. It is quite possible that exotic superconductors behave so because more than one mechanism cooperates. One of arguments for this could be the presence of the untypical isotope effect pointing to the relevance of the phonon-electron interactions in new materials. As is known these materials display strong coupling between phonons and electrons because they are very bad conductors in the normal state and antiferromagnetic Mott insulators when undoped [11].

2 The Model

We are focused on the following Hamiltonian:

$$\begin{aligned}
 H_0 = & \sum_{i \neq j, \sigma} t_{ij}^d d_{i\sigma}^* d_{j\sigma} + (E^d - \mu) \sum_{i\sigma} n_{i\sigma}^d \\
 & - U^d \sum_i n_{i+}^d n_{i-}^d - W \sum_i (d_{i+}^* d_{i-}^* f_{i-} f_{i+} + h.c.) \\
 & + (E^f - \mu) \sum_{i\sigma} n_{i\sigma}^f + U^f \sum_i n_{i+}^f n_{i-}^f \\
 & + V \sum_{i\sigma} (d_{i\sigma}^* f_{i\sigma} + f_{i\sigma}^* d_{i\sigma}) + U^{df} \sum_{i\sigma\sigma'} n_{i\sigma}^f n_{i\sigma'}^d. \quad (2.1)
 \end{aligned}$$

The Hamiltonian describes a system of interacting d- and f-electrons in a solid. $d_{i\sigma}^*$ and $d_{i\sigma}$ are the creation and annihilation operators of an electron from the d-band (the wider one) whereas $f_{i\sigma}^*$ and $f_{i\sigma}$ concern electrons from the narrower f one, respectively. σ denotes the spin of electrons and i and j refer to lattice sites. $n_{i\sigma}^d$ and $n_{i\sigma}^f$ are the number operators of both kinds of electron. The dispersion of the f band was suppressed. E^d and E^f refer to the site energies of both kinds of electron, respectively. V is the conventional on-site hybridization and the parameters $U^d > 0$, U^f and U^{df} are the effective coupling constants of the Coulomb interactions between electrons of the same type and the different ones, respectively. The interaction between d-electrons

is assumed to be attractive leading in this way to appearance of superconductivity in the system. Two remaining ones can be treated arbitrarily, however, it is assumed now that f-electrons repel each other. There is another channel to introduce superconductivity to the system, namely via an on-site exchange of pairs (the pair-hybridization) with opposite spins between bands. The coupling constant of this exchange potential was assumed to be negative. The Hamiltonian (2.1) can be substantiated by the existence of strong local interactions between phonons and electrons in some materials [10, 11, 14]. Such interactions lead to forming polarons which in turn can attract each other. These interacting polarons can be bound into so-called bipolarons. Anyway, superconductivity can be caused by on-site interactions of local phonons with local electrons and its emerging depends really on the magnitude of Coulomb and electron-phonon interactions.

In this paper we will limit ourselves to a simpler case, namely the interband Coulomb interaction and the single-particle hybridization ones in the Hamiltonian above will be dropped. In [16] the interband Coulomb repulsion was taken into account. It turned out that this interaction reduces the superconducting phase with coexisting local pairs and Cooper pairs. Additionally, the following perturbations will be taken into account separately:

$$T_{sf} = \sum_{i \neq j, \sigma} t_{ij}^{sf} f_{i\sigma}^* f_{j\sigma},$$

$$T_{pf} = \sum_{i \neq j} t_{ij}^{pf} f_{i+}^* f_{i-}^* f_{j-} f_{j+}.$$

The first one stands for the hopping of single f-electrons and provides the system with the dispersion of f-electrons making the f-band have the finite width. The second formula is the hopping of pairs of f-electrons. We are interested in the influence of each of the type of the hopping on the critical temperature in the investigated system. Therefore, two Hamiltonians are considered in the paper:

$$H_1 = T_{sf} + H_0 \quad (2.2)$$

and

$$H_2 = T_{pf} + H_0. \quad (2.3)$$

Both kinds of hopping are restricted to the nearest-neighbor case. Additionally, the lattice is assumed to be two-dimensional and the symmetry of the lattice is square. The Hamiltonian H_0 after passing to the momentum space and making use of the so-called BCS approximation in the case of d-electrons takes the following mean field form:

$$H_{0 \text{ red}} = H^d + H^f + LC \quad (2.4)$$

where

$$H^d = \sum_{\mathbf{k}} [\xi_{\mathbf{k}}^d (n_{\mathbf{k}+}^d + n_{\mathbf{k}-}^d) - \tilde{\Delta} (d_{\mathbf{k}+}^* d_{\mathbf{k}-}^* + d_{\mathbf{k}-} d_{\mathbf{k}+})], \quad (2.5)$$

$$H^f = \sum_i [\xi_i^f (n_{i+}^f + n_{i-}^f) + U^f n_{i+}^f n_{i-}^f - \bar{\Delta} (f_{i+}^* f_{i-}^* + f_{i-} f_{i+})] \quad (2.6)$$

and

$$LC = L \frac{\Delta^2}{U^d} + 2L \frac{\bar{\Delta} \rho}{W}.$$

We have obtained the Hamiltonians describing two independent subsystems of d- and f-electrons with the following order parameters:

$$\tilde{\Delta} = \Delta + \rho, \quad (2.7)$$

$$\Delta = \frac{U^d}{L} \sum_{\mathbf{k}} \langle d_{\mathbf{k}+}^* d_{\mathbf{k}-}^* \rangle_{H^d} = \frac{U^d}{L} \sum_{\mathbf{k}} \langle d_{\mathbf{k}-} d_{\mathbf{k}+} \rangle_{H^d}, \quad (2.8)$$

$$\bar{\Delta} = \frac{W}{L} \sum_{\mathbf{k}} \langle d_{\mathbf{k}+}^* d_{\mathbf{k}-}^* \rangle_{H^d} = \frac{W}{L} \sum_{\mathbf{k}} \langle d_{\mathbf{k}-} d_{\mathbf{k}+} \rangle_{H^d} \quad (2.9)$$

and

$$\rho = W \langle f_{i+}^* f_{i-}^* \rangle_{H^f} = W \langle f_{i-} f_{i+} \rangle_{H^f}. \quad (2.10)$$

L is the number of lattice sites. Hamiltonian H^d acts in the momentum space and describes the conventional BCS system whereas H^f concerns the real space and in fact is the sum of on-site contributions. It is worth noting that taking into account of the Coulomb repulsion between f-electrons is more important than the corresponding one in the wider band due to stronger screening effects in it. The averages in the expressions above are taken over the grand canonical ensemble for the corresponding Hamiltonian. The dispersion relation for the d-band is $\varepsilon_{\mathbf{k}}^d = -2t^d (\cos k_x + \cos k_y)$ for $t_{ij}^d = -t^d$, thus $\xi_{\mathbf{k}}^d = E^d + \varepsilon_{\mathbf{k}}^d - \mu$, whereas $\xi^f = E^f - \mu$.

The problem is now reduced to two separate diagonalizations of $H^d = \sum_{\mathbf{k}} H_{\mathbf{k}}^d$ and $H^f = \sum_i H_i^f$ and is quite easy to solve. We furnish the reader with the list of eigenvectors and eigenvalues of H_i^f below only due to two reasons, namely, the solution for $H_{\mathbf{k}}^d$ is widely known besides we will utilize the results below in the perturbation procedure in this paper. Let M_i^f be the subspace of the i th lattice site spanned by the set of the following vectors: $|00\rangle_i$, $|+0\rangle_i$, $|0-\rangle_i$ and $|+-\rangle_i$, which can be written as $(f_{i+}^*)^{n_i} (f_{i-}^*)^{m_i} |00\rangle_i$ with $n_i, m_i = 0, 1$, then

Eigenvector	Eigenvalue
$ +\rangle_i := 00\rangle_i$	ξ^f
$ -\rangle_i := 0-\rangle_i$	ξ^f
$ E\rangle_i := \bar{u} +-\rangle_i - \bar{v}_i 00\rangle_i$	$\xi^f + \frac{U^f}{2} + \bar{E}$
$ G\rangle_i := \bar{u} 00\rangle_i + \bar{v}_i +-\rangle_i$	$\xi^f + \frac{U^f}{2} - \bar{E}$

The eigenvectors are the linear combinations of these vectors, $\bar{u} = \frac{1}{2}(1 + \frac{\xi^f + \frac{U^f}{2}}{\bar{E}})$, $\bar{v} = \frac{1}{2}(1 - \frac{\xi^f + \frac{U^f}{2}}{\bar{E}})$ where $\bar{E} = \sqrt{(\xi^f + \frac{U^f}{2})^2 + \bar{\Delta}^2}$. At this stage both f-electrons themselves and pairs of them are localized on lattice sites and cannot hop from one site to others. This will be possible after taking these effects into account in the form of perturbations.

3 The Free Energy and the Gap Equations

Having found the spectrum of the mean field Hamiltonian (2.4) one can now write down the statistical sum and the gap equations completed with the equation for the average number of electrons per lattice site. The statistical sum written in terms of all the eigenvalues reads

$$Z = e^{-\beta LC} e^{-\beta L \xi^f} 2^L (1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E})^L \times \prod_{\mathbf{k}} e^{-\beta \xi_{\mathbf{k}}^d \cosh^2 \beta \frac{E_{\mathbf{k}}}{2}}. \quad (3.1)$$

The free energy per lattice site is

$$\begin{aligned} \frac{F_0}{L} &= -(\beta L)^{-1} \ln Z \\ &= C + \xi^f - \beta^{-1} \ln 2 (1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}) \\ &\quad + L^{-1} \sum_{\mathbf{k}} \xi_{\mathbf{k}}^d - 2(L\beta)^{-1} \sum_{\mathbf{k}} \ln \cosh \beta \frac{E_{\mathbf{k}}}{2}, \end{aligned} \quad (3.2)$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^d{}^2 + \tilde{\Delta}^2}$. The free energy per lattice site is very useful for determining the order parameters and the chemical potential. It suffices to minimize the free energy per lattice site with respect to these parameters. As a result one obtains the following system of three equations:

$$L^{-1} \frac{\partial F_0}{\partial \rho} = 0 \quad \Rightarrow \quad \bar{\Delta} = \frac{W}{2} \frac{\tilde{\Delta}}{L} \sum_{\mathbf{k}} \frac{\tanh \beta \frac{E_{\mathbf{k}}}{2}}{E_{\mathbf{k}}},$$

$$L^{-1} \frac{\partial F_0}{\partial \Delta} = 0 \quad \Rightarrow \quad \Delta = \frac{U^d}{2} \frac{\tilde{\Delta}}{L} \sum_{\mathbf{k}} \frac{\tanh \beta \frac{E_{\mathbf{k}}}{2}}{E_{\mathbf{k}}}$$

and

$$L^{-1} \frac{\partial F_0}{\partial \Delta} = 0 \Rightarrow \rho = \frac{W\bar{\Delta}}{2\bar{E}} \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}}. \quad (3.3)$$

The set of these equations is to be completed with the equation for the average number of electrons per lattice site

$$\begin{aligned} -L^{-1} \frac{\partial F_0}{\partial \mu} = n \Rightarrow \\ n = 1 - \frac{\xi^f + \frac{U^f}{2}}{\bar{E}} \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}} \\ + L^{-1} \sum_{\mathbf{k}} \left(1 - \frac{\xi_{\mathbf{k}}^d}{E_{\mathbf{k}}} \tanh \beta \frac{E_{\mathbf{k}}}{2} \right) = n^f + n^d, \end{aligned}$$

with

$$n^f = 1 - \frac{\xi^f + \frac{U^f}{2}}{\bar{E}} \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}},$$

where n^f is the average number of f-electrons per lattice site and n^d denotes the average number of d-electrons per lattice site. The equations above are equivalent to those obtained in [10, 14–17] due to the linear relation $\Delta = \frac{U^d}{W} \bar{\Delta}$. Note that the equation for ρ is modified by the presence of the Coulomb repulsion U^f , which is consistent with the corresponding equation, e.g. in [16]. In that paper the pair hopping was taken into account in the equation for ρ as well. Here this factor will be introduced via perturbation theory.

The first two equations above after passing to the thermodynamic limit read

$$\bar{\Delta} = \frac{W}{2} \frac{\tilde{\Delta}}{De} \int_{-\mu}^{De-\mu} \frac{\tanh \beta \frac{E}{2}}{E} d\xi^d, \quad (3.4)$$

and

$$\Delta = \frac{U^d}{2} \frac{\tilde{\Delta}}{De} \int_{-\mu}^{De-\mu} \frac{\tanh \beta \frac{E}{2}}{E} d\xi^d, \quad (3.5)$$

whereas the average number of electrons per lattice site is

$$\begin{aligned} n = 1 - \frac{\xi^f + \frac{U^f}{2}}{\bar{E}} \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}} \\ + \frac{1}{De} \int_{-\mu}^{De-\mu} \left(1 - \frac{\xi^d}{E} \tanh \beta \frac{E}{2} \right) d\xi^d. \end{aligned} \quad (3.6)$$

De is the bandwidth of the d-band while $E = \sqrt{\xi^{d2} + \tilde{\Delta}^2}$. The density of states (DOS) in the d-band was assumed to

be the rectangular one, it is,

$$\rho(\xi_{\mathbf{k}}^d) = \begin{cases} \frac{1}{De}, & \xi_{\mathbf{k}}^d \in (0, De); \\ 0, & \text{otherwise.} \end{cases}$$

This kind of DOS is very frequently used in order to approximate the exact DOS of 2D square lattice systems. After some simple algebra one obtains the following equation:

$$\begin{aligned} \frac{2De}{(U^d + \frac{W^2}{2\bar{E}} \mathcal{F}(\beta, U^f, \bar{\Delta}))} \\ = \int_{-\mu}^{De-\mu} \frac{\tanh \frac{1}{2} \beta \sqrt{\xi^{d2} + \tilde{\Delta}^2}}{\sqrt{\xi^{d2} + \tilde{\Delta}^2}} d\xi^d, \end{aligned}$$

where $\mathcal{F}(\beta, U^f, \bar{\Delta}) = \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}}$. Now having found the equations above one can determine the critical temperature. Putting $\rho = \Delta = \bar{\Delta} = 0$ one arrives at the equation for the inverse critical temperature $\beta_c = \frac{1}{k_B T_c}$, namely

$$\begin{aligned} \frac{2De}{(U^d + \frac{W^2}{2|\xi^f + \frac{U^f}{2}|} \mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0))} \\ = \int_{-\mu}^{De-\mu} \frac{\tanh \frac{1}{2} \beta_c \xi^d}{\xi^d} d\xi^d \end{aligned} \quad (3.7)$$

and the equation for n

$$\begin{aligned} n = 2 - \frac{\xi^f + \frac{U^f}{2}}{|\xi^f + \frac{U^f}{2}|} \mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0) \\ - \frac{2}{\beta_c De} \ln \frac{\cosh \frac{1}{2} \beta_c (De - \mu)}{\cosh \frac{1}{2} \beta_c \mu}. \end{aligned} \quad (3.8)$$

Equation (3.7) suggests the effective increase of the coupling between d-electrons due to the presence of localized pairs of f-electrons. This should lead to elevation of the critical temperature as we shall see below.

For $E^f = \mu = \frac{De}{2}$ both equations reduce to

$$\frac{2De}{(U^d + \frac{W^2}{U^f} \mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0))} = \int_{-\frac{De}{2}}^{\frac{De}{2}} \frac{\tanh \frac{1}{2} \beta_c \xi^d}{\xi^d} d\xi^d$$

and

$$n = 2 - \mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0),$$

with $\mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0) = \frac{1 - e^{-\beta_c U^f}}{3 + e^{-\beta_c U^f}}$. Taking into account two opposite limits $\beta_c U^f \gg 1$ (large U^f and low T_c) and $\beta_c U^f \ll 1$ (small U^f and high T_c), in the former case one

gets

$$\frac{2De}{(U^d + \frac{W^2}{U^f})(\frac{1}{3} - \frac{4}{9}e^{-\beta_c U^f})} = \int_{-\frac{De}{2}}^{\frac{De}{2}} \frac{\tanh \frac{1}{2}\beta_c \xi^d}{\xi^d} d\xi^d$$

and $n = \frac{5}{3} + \frac{4}{9}e^{-\beta_c U^f}$. If U^f and $\beta_c \frac{De}{2}$ get infinite then the critical temperature takes the well known pure BCS result $k_B T_c \approx 1.13 \frac{De}{2} e^{-\frac{De}{U^d}}$ while $n = \frac{5}{3}$. It means that the d-band is half-filled while the f-band is two-thirds full. Of course such a strong repulsion makes the creation of local pairs in the f-band impossible. f-orbitals cannot be occupied by pairs of f-electrons with opposite spins but they are empty or singly occupied. In turn, if the investigated system is at low temperatures but U^f is finite the approximated solution is

$$k_B T_c \approx 1.13 \frac{De}{2} \exp\left(-\frac{De}{U^d + \frac{W^2}{3U^f}}\right),$$

with the proviso that $\beta_c \frac{De}{2}$ is still large. Such a critical temperature is higher than the conventional BCS result. In the $\beta_c U^f \ll 1$ case the equation for this temperature reads

$$\frac{2De}{(U^d + \frac{W^2 \beta_c}{4})} = \int_{-\frac{De}{2}}^{\frac{De}{2}} \frac{\tanh \frac{1}{2}\beta_c \xi^d}{\xi^d} d\xi^d$$

and the average number of electrons per lattice site is

$$n = 2 - \frac{\beta_c U^f}{4}.$$

Thus, in the case of the weak Coulomb repulsion in the f-band one observes the average number of electrons per lattice site to be a little bit smaller than $n = 2$ and the equation for the inverse critical temperature can be written as

$$\frac{1}{\beta_c} = 1.13 \frac{De}{2} \exp\left(-\frac{De}{U^d + \frac{W^2 \beta_c}{4}}\right),$$

if $\beta_c \frac{De}{2}$ is sufficiently large. One can try to solve the equation above by making some simple approximations. First, let us assume that $\frac{W^2 \beta_c}{4} \ll U^d$ then one can apply the expansion $\exp\left(-\frac{De}{U^d + \frac{W^2 \beta_c}{4}}\right) \approx \exp\left(-\frac{De}{U^d}\right)\left(1 + \frac{De}{4}\left(\frac{W}{U^d}\right)^2 \beta_c\right)$. Of course, $\frac{W}{U^d} \ll 1$ is assumed as well. The approximated solution reads

$$k_B T_c \approx \frac{1.13De}{4} e^{-\frac{De}{U^d}} \left(1 + \sqrt{1 + \frac{2}{1.13}\left(\frac{W}{U^d}\right)^2 e^{\frac{De}{U^d}}}\right)$$

and leads to the higher critical temperature than the pure BCS one. If W and U^d are much larger in comparison to De then the expression $\frac{De}{U^d + \frac{W^2 \beta_c}{4}}$ can be regarded as small. In

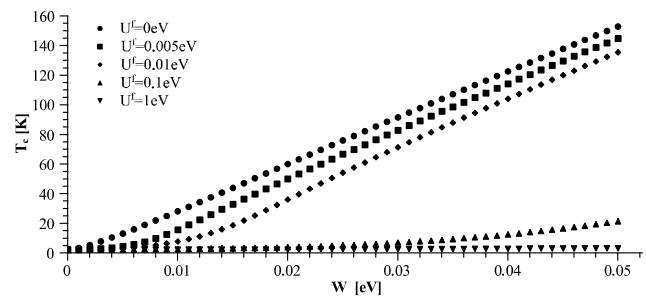


Fig. 1 The dependence of the critical temperature on the coupling constant W for some values of the Coulomb repulsion is depicted. It is seen that the Coulomb repulsion reduces the critical temperature to the BCS value, which is equal to 2.217 K for the parameters used in the paper

this case the expansion $\exp\left(-\frac{De}{U^d + \frac{W^2 \beta_c}{4}}\right) \approx 1 - \frac{De}{U^d + \frac{W^2 \beta_c}{4}}$ is helpful. In terms of that the critical temperature is

$$k_B T_c \approx \frac{1}{2} \frac{1.13De}{1 + \frac{2.26De^2}{W^2}}.$$

This solution points to the higher critical temperature than in the conventional BCS theory as well.

It follows from the considerations above that the pair hybridization increases the critical temperature what is in agreement with the result obtained in [10, 14–17]. Now we can additionally ask about the influence of the Coulomb repulsion on this temperature. This task was achieved numerically for the following set of parameters: $De = 0.05$ eV and $U^d = 0.01$ eV. Moreover, the chemical potential has been fixed in the middle of the d-band, it is $\mu = \frac{De}{2}$. The parameters used in the calculations give the coupling constant of BCS pairing $\frac{U^d}{De} = 0.2$ and the pure BCS critical temperature $T_c = 2.217$ K, thus one has to do with a superconductor in the weak coupling regime. In Fig. 1 the dependence of the critical temperature on the coupling W for different values of the Coulomb repulsion U^f is depicted. The pair hybridization is very effective in increasing the critical temperature but only for weak repulsion between f-electrons. One observes quite strongly increasing functions $T_c(W)$ from the pure BCS value to quite high temperatures; However, if the repulsion is much stronger one can notice curves representing functions that are very weakly increasing. In such a case the formation of local electron pairs is not energetically favorable and lattice sites are either empty or occupied by single f-electrons that cannot be transferred to the d-band due to the lack of a proper channel.

An interesting question is how the location of the f-band with respect to the d-band affects the critical temperature. The same values of U^d , De and μ has been used while $U^f = 0.1$ eV. It turns out that the critical temperature can significantly be affected by one. This is shown in Fig. 2 for three values of W . For $W = 0.001$ eV the change of T_c with respect to the BCS value that equals $T_{cBCS} = 2.217$ K is

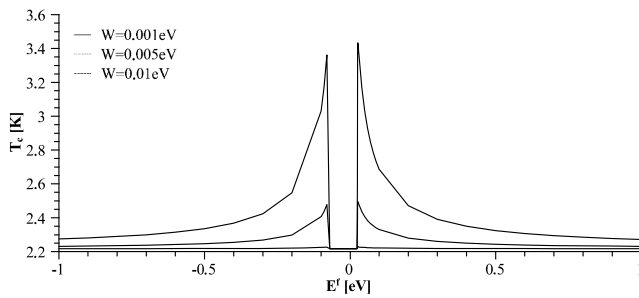


Fig. 2 The dependence of the critical temperature on the position of the f-band with respect to the bottom of the d-band is depicted. There are two peaks at two values of this parameter. The first maximum corresponds to the f-band located below the bottom of the d-band while the second one to the f-band lying very close to the middle of the d-band

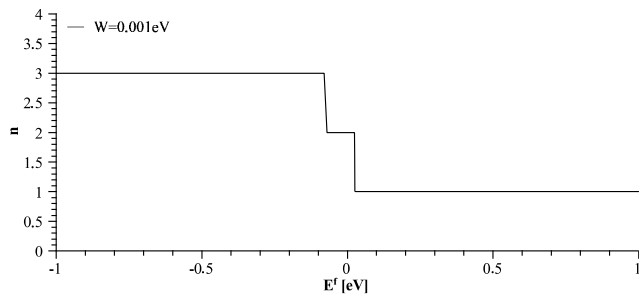


Fig. 3 The average number of electrons per lattice site versus the position of the f-band with respect to the bottom of the d-band. Two steps are visible in the figure. These steps correspond to the inner steep slopes of two peaks seen on Fig. 2

very poor. There are two low maxima at $E^f = -0.08$ eV and $E^f = 0.026$ eV. Shifting the f-level from $-\infty$ upwards one gets the gradual increase of T_c from the BCS value to $T_c = 2.227$ K at $E^f = -0.07$ eV and the rapid fall to the BCS value again. Further shifting does not change this up to the point $E^f = 0.024$ eV where T_c jumps to the value $T_c = 2.228$ K to drop to the BCS value again. Note that d-band has the bandwidth represented by the range (0 eV, 0.05 eV). For the larger value $W = 0.005$ eV the jumps are visibly higher and take place at the same points. The critical temperatures reach $T_c = 2.477$ K and $T_c = 2.493$ K, respectively. Even higher values are reached if $W = 0.01$ eV. These are 3.363 K and 3.434 K for $E^f = -0.08$ eV and $E^f = 0.027$ eV. One can notice that the critical temperature may be significantly elevated if W is sufficiently large and the f-band lies either below the down edge of the d-band or slightly above the center of this band. In Fig. 3 the dependence of the average number of electrons per lattice site for $W = 0.001$ eV is depicted. There is no need to depict the rest of cases because they look likewise. As one can see there are two rapid drops corresponding to two jumps of the critical temperature. When the average number of electrons drops from 3 to 2 the critical temperature falls from

one of two local maximal values to the BCS one. In turn, in the case of the rapid change of this number from 2 to 1 this temperature jumps from the BCS value to the second maximal value. Shifting the f-level further upwards one obtains the constant value of the average number of electrons corresponding to the decreasing critical temperature to the BCS value. It is interesting that the value $n = 2$ is taken for $E^f \in (-0.08 \text{ eV}, 0.024 \text{ eV})$ (half-filled case) and for $E^f = 0.025$ eV one obtains $n \approx 1.67$, which agrees with the analytic result for $\beta_c U^f \gg 1$. For $n = 2$ the critical temperature is equal to the BCS value. For these values of E^f leading to much higher critical temperatures superconductivity is dominated by local electron pairs whereas outside these regions the conventional BCS mechanism is privileged. Note that in [15–17] the authors obtained the BCS result for $U^f = 0$ and $U^f = -\infty$ on shifting the f-level upwards on the energy scale as well.

4 The Effect of Two Kinds of Hopping

In the preceding section the free energy per lattice site has been derived. In this one we would like to investigate the effect of two perturbations separately. These are the hopping of f-electrons and the hopping of pairs of these electrons which are expressed by T_{sf} and T_{pf} . Following [21] one can formulate the total free energy as the expansion up to the second order, namely

$$F = F_0 + \langle H' \rangle_0 + \frac{\beta}{2} \langle H'^2 \rangle_0 - \frac{1}{2} \left\langle \int_0^\beta e^{wH_0} H' e^{-wH_0} H' dw \right\rangle_0. \quad (4.1)$$

H' stands for arbitral perturbation. Note that actually the calculations will be made in the subspace of f-electrons because the operators representing two types of hopping act in this subspace only. Having in mind this remark one can write the unperturbed free energy F_0^f down

$$F_0^f = \text{Tr} e^{-\beta H^f} = L \xi^f - \beta^{-1} L \ln 2 (1 + e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}). \quad (4.2)$$

The Hamiltonian H^f acts in $\bigotimes_{i=1}^L M_i^f$ spanned by the vectors $(f_{1+}^*)^{n_1} (f_{1-}^*)^{m_1} |00\rangle_1 \otimes \dots \otimes (f_{L+}^*)^{n_L} (f_{L-}^*)^{m_L} |00\rangle_L$. The periodic boundary conditions were adopted here. In order to make further calculations let us define the density matrix

$$\rho^f := \bigotimes_{i=1}^L \rho_i^f, \quad (4.3)$$

where

$$\rho_i^f := \frac{e^{-\beta\xi^f}}{Z^f} (|+\rangle_{ii}\langle+| + |-\rangle_{ii}\langle-|) \\ + \frac{e^{-\beta(\xi^f + \frac{U^f}{2} + \bar{E})}}{Z^f} |E\rangle_{ii}\langle E| \\ + \frac{e^{-\beta(\xi^f + \frac{U^f}{2} - \bar{E})}}{Z^f} |G\rangle_{ii}\langle G|$$

with

$$Z^f := 2e^{-\beta\xi^f} (1 + e^{-\beta\frac{U^f}{2}} \cosh \beta\bar{E}).$$

The symbol $|A\rangle\langle A|$ denotes the projection operator on a state $|A\rangle$. Note that $\text{Tr} \rho^f = \prod_{i=1}^L \text{Tr} \rho_i^f = 1$. Next, if one looks at the structure of the operators T_{sf} and T_{pf} then it will be obvious that they connect two neighboring sites i and $i+1$. Let us write these operators in the following forms:

$$T_{\text{sf}} = -t^{\text{sf}} \sum_{\sigma} \sum_{i=1}^L (f_{i\sigma}^* f_{i+1\sigma} + f_{i+1\sigma}^* f_{i\sigma})$$

and

$$T_{\text{pf}} = -t^{\text{pf}} \sum_{i=1}^L (f_{i+}^* f_{i-}^* f_{i+1-} f_{i+1+} + f_{i+1+}^* f_{i+1-}^* f_{i-} f_{i+}).$$

Now let us calculate the correction to the free energy due to the pair hopping up to the first order. We deal with the 2D-system and in fact all operators should be denoted with a double index whereas the sums should be double. However, for simplicity the abbreviated notation was used. More details are included in Appendix A. Thus

$$\langle T_{\text{pf}} \rangle_{H^d} = -t^{\text{pf}} \sum_{i=1}^L \text{Tr} \rho^f (f_{i+}^* f_{i-}^* f_{i+1-} f_{i+1+} \\ + f_{i+1+}^* f_{i+1-}^* f_{i-} f_{i+}) \\ = -t^{\text{pf}} \sum_{i=1}^L \text{Tr} \rho_i^f \otimes \rho_{i+1}^f (f_{i+}^* f_{i-}^* f_{i+1-} f_{i+1+} \\ + f_{i+1+}^* f_{i+1-}^* f_{i-} f_{i+}). \quad (4.4)$$

Note that $\rho_i^f \otimes \rho_{i+1}^f$ was left under the trace only since the rest of the factors were traced out to give the unity. This operator takes the following form:

$$\rho_i^f \otimes \rho_{i+1}^f = \frac{e^{-2\beta\xi^f}}{Z^{f2}} [|+\rangle_i \otimes |+\rangle_{i+1} \langle+| \otimes \langle+| \\ + |+\rangle_i \otimes |-\rangle_{i+1} \langle-| \otimes \langle+| \\ + e^{-\beta(\frac{U^f}{2} - \bar{E})} |+\rangle_i \otimes |G\rangle_{i+1} \langle G| \otimes \langle+|$$

$$+ e^{-\beta(\frac{U^f}{2} + \bar{E})} |+\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes \langle+| \\ + |-\rangle_i \otimes |+\rangle_{i+1} \langle+| \otimes \langle-| \\ + |-\rangle_i \otimes |-\rangle_{i+1} \langle-| \otimes \langle-| \\ + e^{-\beta(\frac{U^f}{2} - \bar{E})} |-\rangle_i \otimes |G\rangle_{i+1} \langle G| \otimes \langle-| \\ + e^{-\beta(\frac{U^f}{2} + \bar{E})} |-\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes \langle-| \\ + e^{-\beta(\frac{U^f}{2} - \bar{E})} |G\rangle_i \otimes |+\rangle_{i+1} \langle+| \otimes \langle G| \\ + e^{-\beta(\frac{U^f}{2} - \bar{E})} |G\rangle_i \otimes |-\rangle_{i+1} \langle-| \otimes \langle G| \\ + e^{-2\beta(\frac{U^f}{2} - \bar{E})} |G\rangle_i \otimes |G\rangle_{i+1} \langle G| \otimes \langle G| \\ + e^{-\beta U^f} |G\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes \langle G| \\ + e^{-\beta(\frac{U^f}{2} + \bar{E})} |E\rangle_i \otimes |+\rangle_{i+1} \langle+| \otimes \langle E| \\ + e^{-\beta(\frac{U^f}{2} + \bar{E})} |E\rangle_i \otimes |-\rangle_{i+1} \langle-| \otimes \langle E| \\ + e^{-\beta U^f} |E\rangle_i \otimes |G\rangle_{i+1} \langle G| \otimes \langle E| \\ + e^{-2\beta(\frac{U^f}{2} + \bar{E})} |E\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes \langle E|].$$

Finally, making use of the expression above one yields

$$\text{cor}_{\text{pf}} = \langle T_{\text{pf}} \rangle_{H^d} = -t^{\text{pf}} z L (2\bar{u}^2 \bar{v}^2 f_{p1} + (\bar{u}^2 - \bar{v}^2)^2 f_{p2}), \quad (4.5)$$

where z is the coordination number which for a 2D-system equals 4 and

$$f_{p1} := \frac{1}{4} \frac{e^{-\beta U^f} \cosh 2\beta\bar{E}}{M^{f2}}, \quad f_{p2} := \frac{1}{4} \frac{e^{-\beta U^f}}{M^{f2}},$$

$$M^f := 1 + e^{-\beta\frac{U^f}{2}} \cosh \beta\bar{E}.$$

Details of the calculations are in Appendix A.

The first order corrections due to the hopping of single particles and $\langle T_{\text{sf}} \rangle_{H^d}^2$ vanish and there is a need to find next terms. We are going to focus on the second order which is quite complex and details of the calculation are presented in Appendix B. The final result is

$$\text{cor}_{\text{sf}} = -\frac{1}{2} \left\langle \int_0^\beta e^{wH^f} T_{\text{sf}} e^{-wH^f} T_{\text{sf}} dw \right\rangle_{H^d} \\ = -t_{\text{sf}}^2 z L \left[4\bar{u}^2 \bar{v}^2 \left(\frac{f_{s1}}{U^f - 2\bar{E}} + 2 \frac{f_{s2}}{\bar{E}} - \frac{f_{s3}}{U^f + 2\bar{E}} \right) \right. \\ \left. + 2(\bar{u}^2 - \bar{v}^2)^2 \left(\frac{f_{s4}}{U^f} + \beta f_{s5} \right) \right], \quad (4.6)$$

where

$$f_{s1} := \frac{1}{4} \frac{1 - e^{-2\beta(\frac{U^f}{2} - \bar{E})}}{M^{f2}}, \quad f_{s2} := \frac{1}{4} \frac{e^{-\beta\frac{U^f}{2}} \sinh \beta\bar{E}}{M^{f2}},$$

$$f_{s3} := \frac{1}{4} \frac{1 - e^{-\beta U^f}}{M f^2},$$

$$f_{s4} := \frac{1}{4} \frac{-1 + e^{-2\beta(\frac{U^f}{2} + \bar{E})}}{M f^2}, \quad f_{s5} := \frac{1}{4} \frac{e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E}}{M f^2}.$$

Now having found the corrections cor_{pf} and cor_{sf} one can incorporate them into the free energy of the f-subsystem per lattice site. It yields

$$\frac{F_{Tp}}{L} = \frac{F_0^d}{L} + \frac{F_p^f}{L} + C = \frac{F_0^d}{L} + \frac{F_0^f}{L} + \frac{cor_{pf}}{L} + C$$

and

$$\frac{F_{Ts}}{L} = \frac{F_0^d}{L} + \frac{F_s^f}{L} + C = \frac{F_0^d}{L} + \frac{F_0^f}{L} + \frac{cor_{sf}}{L} + C,$$

where $\frac{F_0^d}{L} = L^{-1} \sum_{\mathbf{k}} \xi_{\mathbf{k}}^d - 2(L\beta)^{-1} \sum_{\mathbf{k}} \ln \cosh \beta \frac{E_{\mathbf{k}}}{2}$. In order to find the equation for the critical temperature for both cases one has to determine the gaps equations from the conditions below:

$$\frac{\partial}{\partial \Delta} \frac{F_{Tn}}{L} = 0, \quad \frac{\partial}{\partial \rho} \frac{F_{Tn}}{L} = 0, \quad \frac{\partial}{\partial \Delta} \frac{F_{Tn}}{L} = 0,$$

where $n = p, s$.

In fact the first two of them are exactly the same as in Sect. 3; however, the third one is transformed to a form with correction terms and after some algebra it leads to the following equation for β_c :

$$\begin{aligned} & \frac{2De}{(U^d + \frac{W^2}{2|\xi^f + \frac{U^f}{2}|} \mathcal{F}(\beta_c, U^f, \bar{\Delta} = 0) - \frac{W^2}{2} c\tilde{or}_{nf}|_{\bar{\Delta}=0})} \\ &= \int_{-\mu}^{De-\mu} \frac{\tanh \frac{1}{2} \beta_c \xi^d}{\xi^d} d\xi^d, \end{aligned} \quad (4.7)$$

where

$$c\tilde{or}_{pf}|_{\bar{\Delta}=0} \approx -\frac{2}{9} \frac{t^{pf} z}{U^f{}^2}, \quad (4.8)$$

$$\begin{aligned} c\tilde{or}_{sf}|_{\bar{\Delta}=0} &\approx -\frac{2}{9} \frac{t^{sf2} z}{U^f{}^3} (2 - 2\beta_c U^f + \beta_c^2 U^f{}^2) \\ &\approx -\frac{2}{9} \frac{t^{sf2} z}{U^f} \beta_c^2. \end{aligned} \quad (4.9)$$

The two expressions above have been obtained for $E^f = \mu = \frac{De}{2}$ and $\beta^c U^f \gg 1$. The reader interested in details of the calculations is referred to Appendix C. Equation (4.7) is solved numerically for $E^f = \mu = \frac{De}{2}$ with making use of (4.8) and (4.9). The bandwidth is $De = 0.05$ eV while $U^d = 0.01$ eV, $U^f = 1$ eV and $W = 0.005$ eV. It is obvious

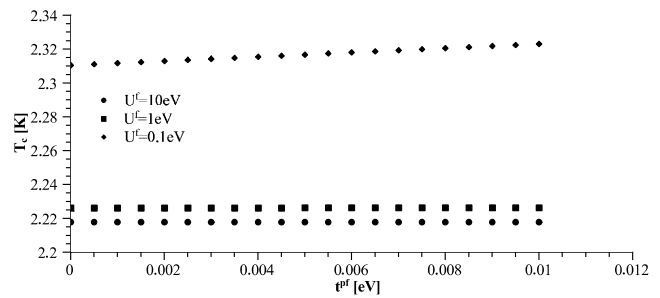


Fig. 4 The dependence of the critical temperature on the pair hopping integral t^{pf} for some values of the Coulomb repulsion is depicted. It is seen that the Coulomb repulsion hampers the increase of the critical temperature from the BCS value which is equal to 2.217 K for the parameters used in the paper. This kind of the hopping is not too efficient in increasing this temperature

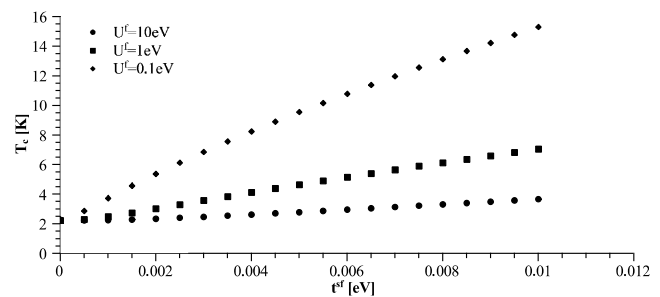


Fig. 5 The dependence of the critical temperature on the single-polaron hopping integral t^{sf} for some values of the Coulomb repulsion is depicted. It is seen that the Coulomb repulsion weakens the increase of the critical temperature from the BCS value which is equal to 2.217 K for the parameters used in the paper. However, this kind of the hopping is far more efficient in rising this temperature than the pair hopping

from Figs. 4 and 5 that the hopping of bipolarons is not as effective in the increase of the critical temperature as that is in the case of the hopping of single polarons. One can notice the effect of the Coulomb repulsion on both cases. If it is sufficiently strong the lines represent functions of hopping integrals which are very weakly increasing. This especially concerns the system with the pair hopping. But even if this interaction is significantly weaker one observes a modest effect of the hopping of bipolarons on the increase of the critical temperature despite the fact that this hopping is incorporated as the correction of the first order. Of course, in [17] it was found that the pair hopping increased the critical temperature what is in agreement with the results obtained in this paper. The next figures, Figs. 6 and 7, show the dependence of the critical temperatures on the exchange pair coupling constant for several values of the hopping integrals. Here the influence of the hopping of local pairs on the critical temperature is found to be quite poor in contrast to the single-polaron hopping that turns out to be much more efficient in elevating this temperature. A possible explanation

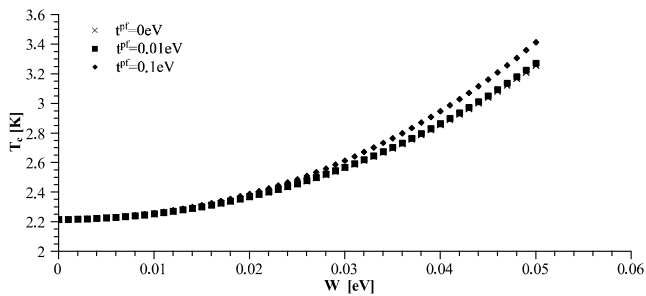


Fig. 6 The dependence of the critical temperature on the coupling constant W for some values of the pair hopping integral t^{pf} is depicted. The critical temperature evidently increases with W , however, the hopping of pairs exerts rather poor effect on this temperature

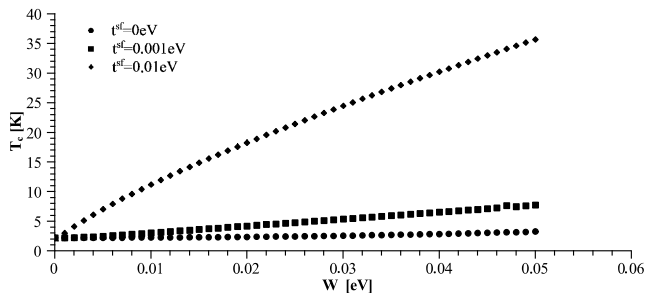


Fig. 7 The dependence of the critical temperature on the coupling constant W for some values of the single-polaron hopping integral t^{sf} is depicted. The hopping of single polarons as well as the pair-exchange potential significantly increase the critical temperature

of this can be the magnitude of the effective mass which is much larger in the case of bipolarons and leads to smaller bandwidth than in the case of single polarons.

Magnetic correlations caused by the single-electron hopping stand for a separate problem. It is widely known that the Hubbard model in the limit of strong on-site Coulomb repulsion displays the antiferromagnetic correlations which lead to the long-range antiferromagnetic order in a half-filled band. In our case these correlations are present as well and compete with superconductivity in the narrower band. They become especially important when U^f gets sufficiently strong to significantly weaken superconductivity. Electron pairs are broken in the f-band and there appears the tendency that f-orbitals at adjacent lattice sites are occupied by single electrons with opposite spins. Additionally, if the system is half-filled then superconductivity in the f-band is completely suppressed to give way to the antiferromagnetic order. In such a case in the wider band the BCS superconductivity can survive while superconductivity in the f-band due to the pair hybridization and pair hopping is absent. The BCS interaction in the wider band is absent in earlier papers [10, 14–17] and in such a case the antiferromagnetic correlations would destroy superconductivity in the system. This issue was briefly analyzed in [17] as well.

Of course, it would be the best to investigate the coexistence of two kinds of hopping in the system, however, this is a much more complicated task. Besides, dealing with them separately one can make some comparison between them. Taking into account both of them acting together in the system will be a subject of future investigations.

5 Conclusions

The influence of several factors on the critical temperature of a two-band superconducting system with BCS pairs of d-electrons and local f-electron pairs was investigated. Such local pairs called bipolarons as well were induced in the f-electron band via the pair-exchange potential coming from an interaction between local phonons and electrons from both bands. These factors were as follows: the local Coulomb repulsion between f-electrons, the position of the f-band with respect to the bottom of the d-band, the hopping of single polarons and the hopping of their pairs. The last two were investigated independently. It turned out that in all cases the Coulomb repulsion in the f-band lowered the critical temperature and acted as a pair-breaker in the f-band, as was very intuitive. If this interaction is sufficiently strong then it will prevent polarons from forming local pairs. Additionally, if the Coulomb interaction is stronger than the value of the bandwidth of the f-band and the system is half-filled, then f-orbitals have the tendency to be occupied by single f-electrons. When the f-orbitals become occupied in that way superconductivity can survive in the d-band with the pure BCS critical temperature. There can be no charge transfer in the form of electron pairs from the f-band due to too strong Coulomb repulsion.

The effect of both kinds of hopping was investigated by making use of perturbation theory. It was done for both of them separately. The conventional hopping of single polarons proved to be much more efficient in making the critical temperature higher than the pair-hopping. This can be due to the higher effective mass of local pairs. The next step in investigations will be taking into account the interplay of two kinds of hopping and the influence of the position of the f-band with respect to the bottom of the d-band.

The effect of the position of the f-band on the critical temperature proved to be very interesting on its own. At two values of this parameter the critical temperature has a jump. These jumps are high if the coupling constant of the pair exchange potential is sufficiently large. This can be described as follows: the critical temperature tends asymptotically to the BCS value when the f-band is shifted towards $-\infty$ but as the f-band is getting closer to the bottom of the d-band this temperature becomes higher and higher up to the mo-

ment when the first local maximum is reached. The critical temperature drops rapidly to get the BCS value again. This value is retained if the position of the f-level is below the center of the d-band. If this level gets the center of the d-band the critical temperature jumps. Further shifting the f-level to ∞ brings about the decrease of the critical temperature to the BCS value. This purely chemical process can lead to quite high values of the critical temperatures and is accompanied by the change of the average number of f-electrons. The investigated system can be treated as a concentrated alloy or a compound in which f-electrons come from atoms of an element introduced into that.

The paper deals with the critical temperature and possible factors influencing it. Other properties of this system are certainly affected by these factors as well. The ground state, the energetic gaps, thermodynamics and electromagnetic properties were already investigated to a large extent [15–17]. However, it could be worthwhile to examine them in the presence of both hoppings. The next question is if there exist materials displaying this untypical behavior of the critical temperature with reference to the position of the f-level. The papers [15–17] point clearly to the doped bismuthates $\text{Ba}_{1-x}\text{K}_x\text{BiO}_3$ and $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$. These chemical complexes possess a pseudogap in the excitation spectrum that can be observed in photoemission experiments [22–25]. It is widely accepted that the presence of incoherent electron pairs above the critical temperature leads to such a pseudogap. The pseudogap appears at some temperature higher than the critical temperature calculated in the frame of the mean field method. It happens that way since the process of pairing in unconventional superconductors can be independent of the phase coherence unlike in conventional ones. In the papers [17, 26] the Kosterlitz–Thouless theory was invoked in order to incorporate this pairing temperature to the considerations. Undoubtedly, the system investigated in this paper is a BCS superconductor with an additional mechanism leading to higher critical temperatures. It is quite possible that such a mixed mechanism is responsible for higher values of the transition temperature. Note that if the f-level is far from the d-band at energetic scale the behavior of the investigated system is dominated by the BCS mechanism and the contribution of coherent local pairs is poor. The condensate of local pairs is much more important in the regions of two peaks and is responsible for the elevation of T_c .

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Appendix A

Our goal is to derive the expression (4.5). To this end let us start with (4.4),

$$\begin{aligned} \text{cor}_{\text{pf}} &= -t^{\text{pf}} \sum_{i=1}^L \text{Tr} \rho_i^f \otimes \rho_{i+1}^f (f_{i+}^* f_{i-}^* f_{i+1-} f_{i+1+} \\ &\quad + f_{i+1+}^* f_{i+1-}^* f_{i-} f_{i+}) \\ &= -t^{\text{pf}} \frac{e^{-2\beta\xi^f}}{Z^f} \sum_{i=1}^L \text{Tr} [(e^{-2\beta(\frac{U^f}{2} - \bar{E})} |G\rangle_i \\ &\quad \otimes |G\rangle_{i+1} \langle G| \otimes |G\rangle_i \\ &\quad + e^{-\beta U^f} |G\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes |G\rangle_i \\ &\quad + e^{-\beta U^f} |E\rangle_i \otimes |G\rangle_{i+1} \langle G| \otimes |E\rangle_i \\ &\quad + e^{-2\beta(\frac{U^f}{2} + \bar{E})} |E\rangle_i \otimes |E\rangle_{i+1} \langle E| \otimes |E\rangle_i) \\ &\quad \times (f_{i+}^* f_{i-}^* f_{i+1-} f_{i+1+} + f_{i+1+}^* f_{i+1-}^* f_{i-} f_{i+})] \\ &= -t^{\text{pf}} \frac{e^{-2\beta\xi^f}}{Z^f} \sum_{i=1}^L \text{Tr} [(e^{-2\beta(\frac{U^f}{2} - \bar{E})} \bar{u}\bar{v}(|G\rangle_i \\ &\quad \otimes |G\rangle_{i+1} \langle -+ | \otimes |00\rangle \\ &\quad + |G\rangle_i \otimes |G\rangle_{i+1} \langle 00| \otimes | -+ |) \\ &\quad + e^{-\beta U^f} (-\bar{v}^2 |G\rangle_i \otimes |E\rangle_{i+1} \langle -+ | \otimes |00\rangle \\ &\quad + \bar{u}^2 |G\rangle_i \otimes |E\rangle_{i+1} \langle 00| \otimes | -+ |) \\ &\quad + e^{-\beta U^f} (\bar{u}^2 |E\rangle_i \otimes |G\rangle_{i+1} \langle -+ | \otimes |00\rangle \\ &\quad - \bar{v}^2 |E\rangle_i \otimes |G\rangle_{i+1} \langle 00| \otimes | -+ |) \\ &\quad - e^{-2\beta(\frac{U^f}{2} + \bar{E})} \bar{v}\bar{u}(|E\rangle_i \otimes |E\rangle_{i+1} \langle -+ | \\ &\quad \otimes |00\rangle + |E\rangle_i \otimes |E\rangle_{i+1} \langle 00| \otimes | -+ |)]. \end{aligned}$$

One should note that the sum in expression above is an abbreviation. This means we have a summation over all neighboring lattice sites. In general in a n-dimensional system every lattice site has $z = 2n$ closest neighbors. Here, for the two-dimensional system one deals with a double sum. For a 2-D system one has

$$\begin{aligned} T_{\text{sf}} &= -t^{\text{sf}} \sum_{\sigma} \sum_{i=1}^{\sqrt{L}} \sum_{j=1}^{\sqrt{L}} (f_{ji\sigma}^* f_{ji+1\sigma} + f_{ji+1\sigma}^* f_{ji\sigma} \\ &\quad + f_{ji\sigma}^* f_{j+1i\sigma} + f_{j+1i\sigma}^* f_{ji\sigma}) \end{aligned}$$

and

$$T_{\text{pf}} = -t^{\text{pf}} \sum_{i=1}^{\sqrt{L}} \sum_{j=1}^{\sqrt{L}} (f_{ji+}^* f_{ji-}^* f_{ji+1-} f_{ji+1+}$$

$${}_i\langle 6|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|6\rangle_i = 0,$$

$${}_i\langle 6|T_{\text{sfi}}|14\rangle_i = {}_i\langle 14|T_{\text{sfi}}|6\rangle_i = -2\bar{u}\bar{v},$$

$$\forall m \in \{8, \dots, 16\} \setminus \{8, 9\}$$

$${}_i\langle 7|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|7\rangle_i = 0,$$

$${}_i\langle 7|T_{\text{sfi}}|8\rangle_i = {}_i\langle 8|T_{\text{sfi}}|7\rangle_i = \bar{u}^2 - \bar{v}^2 \quad \text{and}$$

$${}_i\langle 7|T_{\text{sfi}}|9\rangle_i = {}_i\langle 9|T_{\text{sfi}}|7\rangle_i = -\bar{u}^2 + \bar{v}^2,$$

$$\forall m \in \{9, \dots, 16\} \setminus \{12\}$$

$${}_i\langle 8|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|8\rangle_i = 0,$$

$${}_i\langle 8|T_{\text{sfi}}|12\rangle_i = {}_i\langle 12|T_{\text{sfi}}|8\rangle_i = -2\bar{u}\bar{v},$$

$$\forall m \in \{10, \dots, 16\} \setminus \{12\}$$

$${}_i\langle 9|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|9\rangle_i = 0,$$

$${}_i\langle 9|T_{\text{sfi}}|12\rangle_i = {}_i\langle 12|T_{\text{sfi}}|9\rangle_i = 2\bar{u}\bar{v},$$

$$\forall m \in \{11, \dots, 16\} \quad {}_i\langle 10|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|10\rangle_i = 0,$$

$$\forall m \in \{12, \dots, 16\} \quad {}_i\langle 11|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|11\rangle_i = 0,$$

$$\forall m \in \{13, \dots, 16\} \quad {}_i\langle 12|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|12\rangle_i = 0,$$

$$\text{for } m = 14 \text{ and } m = 16$$

$${}_i\langle 13|T_{\text{sfi}}|m\rangle_i = {}_i\langle m|T_{\text{sfi}}|13\rangle_i = 0,$$

$${}_i\langle 13|T_{\text{sfi}}|15\rangle_i = {}_i\langle 15|T_{\text{sfi}}|13\rangle_i = \bar{v}^2 - \bar{u}^2,$$

$${}_i\langle 14|T_{\text{sfi}}|15\rangle_i = {}_i\langle 15|T_{\text{sfi}}|14\rangle_i = 0,$$

$${}_i\langle 14|T_{\text{sfi}}|16\rangle_i = {}_i\langle 16|T_{\text{sfi}}|14\rangle_i = \bar{v}^2 - \bar{u}^2,$$

$${}_i\langle 15|T_{\text{sfi}}|16\rangle_i = {}_i\langle 16|T_{\text{sfi}}|15\rangle_i = 0.$$

Having the matrix elements at disposal one can resort to finding the denominators $E_n - E_m$ in (B.1). These are as follows:

$$E_1 - E_8 = E_1 - E_9 = U^f - 2\bar{E},$$

$$E_2 - E_{15} = E_3 - E_{16} = E_5 - E_{13} = E_6 - E_{14} = -2\bar{E},$$

$$E_8 - E_{12} = E_9 - E_{12} = -U^f - 2\bar{E},$$

$$E_4 - E_8 = E_4 - E_9 = E_7 - E_8 = E_7 - E_9 = U^f,$$

$$E_3 - E_6 = E_2 - E_5 = E_{13} - E_{15} = E_{14} - E_{16} = 0.$$

Notice that some of them equal zero, in spite of there being no singularities in the correction terms since the ratios $\frac{e^{\beta(E_n - E_m)} - 1}{E_n - E_m}$ converge to β if $E_n - E_m \rightarrow 0$. Now it remains to collect all terms in (B.1) to obtain the formula (4.6).

Appendix C

To calculate $c\tilde{r}_{\text{pf}}|_{\bar{\Delta}=0}$ and $c\tilde{r}_{\text{sf}}|_{\bar{\Delta}=0}$ is a tedious task. Let us start with the former expression. The following derivatives

are necessary:

$$\frac{\partial f_{p1}}{\partial \bar{\Delta}} = \frac{1}{2}\beta e^{-\beta U^f} \frac{\bar{\Delta}}{\bar{E}} \times \left[\frac{\sinh 2\beta \bar{E}}{M^f{}^2} - \frac{e^{-\beta \frac{U^f}{2}} \cosh 2\beta \bar{E} \sinh \beta \bar{E}}{M^f{}^3} \right],$$

$$\frac{\partial f_{p2}}{\partial \bar{\Delta}} = -\frac{1}{2}\beta e^{-3\beta \frac{U^f}{2}} \frac{\bar{\Delta}}{\bar{E}} \frac{\sinh \beta \bar{E}}{M^f{}^3}.$$

Additionally, knowing that $\bar{u}^2 - \bar{v}^2 = \frac{E^f - \mu + \frac{U^f}{2}}{\bar{E}}$ and $\bar{u}\bar{v} = \frac{1}{2} \frac{\bar{\Delta}}{\bar{E}}$, one obtains

$$\frac{\partial (\bar{u}^2 - \bar{v}^2)^2}{\partial \bar{\Delta}} = -2\bar{\Delta} \frac{(E^f - \mu + \frac{U^f}{2})^2}{\bar{E}^4},$$

$$\frac{\partial \bar{u}^2 \bar{v}^2}{\partial \bar{\Delta}} = \frac{1}{2} \frac{\bar{\Delta}}{\bar{E}^2} \left(1 - \frac{\bar{\Delta}^2}{\bar{E}^2} \right).$$

Thus

$$\begin{aligned} \frac{1}{L} \frac{\partial \text{cor}_{\text{pf}}}{\partial \bar{\Delta}} &= -t^{\text{pf}} z \left[2 \left(\frac{\partial \bar{u}^2 \bar{v}^2}{\partial \bar{\Delta}} f_{p1} + \bar{u}^2 \bar{v}^2 \frac{\partial f_{p1}}{\partial \bar{\Delta}} \right) \right. \\ &\quad \left. + \frac{\partial (\bar{u}^2 - \bar{v}^2)^2}{\partial \bar{\Delta}} f_{p2} + (\bar{u}^2 - \bar{v}^2)^2 \frac{\partial f_{p2}}{\partial \bar{\Delta}} \right] \\ &= \bar{\Delta} c\tilde{r}_{\text{pf}}, \end{aligned}$$

where

$$\begin{aligned} c\tilde{r}_{\text{pf}} &= -\frac{1}{2} \frac{t^{\text{pf}} z e^{-\beta U^f}}{\bar{E}^2 M^f} \left[\frac{1}{2} \left(1 - \frac{\bar{\Delta}^2}{\bar{E}^2} \right) \cosh 2\beta \bar{E} \right. \\ &\quad \left. + \frac{1}{2} \beta \frac{\bar{\Delta}^2}{\bar{E}} \left(\sinh 2\beta \bar{E} - \frac{e^{-\beta \frac{U^f}{2}} \cosh 2\beta \bar{E} \sinh \beta \bar{E}}{M^f} \right) \right. \\ &\quad \left. - \frac{(E^f - \mu + \frac{U^f}{2})^2}{\bar{E}^2} \right. \\ &\quad \left. - \beta \frac{(E^f - \mu + \frac{U^f}{2})^2}{\bar{E}} \frac{e^{-\beta \frac{U^f}{2}} \sinh \beta \bar{E}}{M^f} \right]. \quad (\text{C.1}) \end{aligned}$$

For simplicity let us take $E^f = \mu = \frac{D\epsilon}{2}$ on. It is easy to show that under proviso $\beta_c U^f \gg 1$ the expression (C.1) for $\bar{\Delta} = 0$ reduces to (4.8).

Similarly, $c\tilde{r}_{\text{sf}}|_{\bar{\Delta}=0}$ can be found with the help of

$$\begin{aligned} \frac{\partial f_{s1}}{\partial \bar{\Delta}} &= -\frac{1}{2}\beta e^{-\beta U^f} \frac{\bar{\Delta}}{\bar{E}} \\ &\quad \times \left[\frac{e^{2\beta \bar{E}}}{M^f{}^2} + \frac{e^{\beta \frac{U^f}{2}} (1 - e^{-\beta U^f}) \sinh \beta \bar{E}}{M^f{}^3} \right], \end{aligned}$$

$$\begin{aligned}
\frac{\partial f_{s2}}{\partial \Delta} &= \frac{1}{4} \beta e^{-\beta \frac{U^f}{2}} \frac{\bar{\Delta}}{E} \left[\frac{\cosh \beta \bar{E}}{M f^2} - 2 \frac{e^{-\beta \frac{U^f}{2}} \sinh^2 \beta \bar{E}}{M f^3} \right], \\
\frac{\partial f_{s3}}{\partial \Delta} &= -\frac{1}{2} \beta e^{-\beta \frac{U^f}{2}} \frac{\bar{\Delta}}{E} \left[\frac{(1 - e^{-\beta U^f}) \sinh \beta \bar{E}}{M f^3} \right], \\
\frac{\partial f_{s4}}{\partial \Delta} &= -\frac{1}{2} \beta e^{-\beta U^f} \frac{\bar{\Delta}}{E} \\
&\quad \times \left[\frac{e^{-2\beta \bar{E}}}{M f^2} + \frac{e^{\beta \frac{U^f}{2}} (-1 + e^{-\beta(U^f + 2\bar{E})}) \sinh \beta \bar{E}}{M f^3} \right], \\
\frac{\partial f_{s5}}{\partial \Delta} &= \frac{1}{4} \beta e^{-\beta \frac{U^f}{2}} \frac{\bar{\Delta}}{E} \\
&\quad \times \left[\frac{\sinh \beta \bar{E}}{M f^2} - 2 \frac{e^{-\beta \frac{U^f}{2}} \cosh \beta \bar{E} \sinh \beta \bar{E}}{M f^3} \right].
\end{aligned}$$

Moreover, the following derivatives are necessary:

$$\begin{aligned}
\frac{\partial}{\partial \Delta} \frac{1}{U^f - 2\bar{E}} &= \frac{2}{(U^f - 2\bar{E})^2} \frac{\bar{\Delta}}{E}, \\
\frac{\partial}{\partial \Delta} \frac{1}{U^f + 2\bar{E}} &= -\frac{2}{(U^f + 2\bar{E})^2} \frac{\bar{\Delta}}{E}, \quad \frac{\partial}{\partial \Delta} \frac{1}{E} = -\frac{\bar{\Delta}}{E^3}.
\end{aligned}$$

Additionally $\frac{\partial(\bar{u}^2 - \bar{v}^2)}{\partial \Delta}$ and $\frac{\partial \bar{u}^2 \bar{v}^2}{\partial \Delta}$ are indispensable but they have been already calculated. Having found the expressions above one can write down

$$\begin{aligned}
\frac{1}{L} \frac{\partial cor_{pf}}{\partial \Delta} &= -t^{sf2} z \left[4 \frac{\partial \bar{u}^2 \bar{v}^2}{\partial \Delta} \left(\frac{f_{s1}}{U^f - 2\bar{E}} + 2 \frac{f_{s2}}{E} \right. \right. \\
&\quad \left. \left. - \frac{f_{s3}}{U^f + 2\bar{E}} \right) + 4 \bar{u}^2 \bar{v}^2 \left(\frac{1}{U^f - 2\bar{E}} \frac{\partial f_{s1}}{\partial \Delta} \right. \right. \\
&\quad \left. \left. + 2 \frac{1}{E} \frac{\partial f_{s2}}{\partial \Delta} - \frac{1}{U^f + 2\bar{E}} \frac{\partial f_{s3}}{\partial \Delta} \right. \right. \\
&\quad \left. \left. + f_{s1} \frac{\partial}{\partial \Delta} \frac{1}{U^f - 2\bar{E}} + 2 f_{s2} \frac{\partial}{\partial \Delta} \frac{1}{E} \right. \right. \\
&\quad \left. \left. - f_{s3} \frac{\partial}{\partial \Delta} \frac{1}{U^f + 2\bar{E}} \right) + 2 \frac{\partial(\bar{u}^2 - \bar{v}^2)^2}{\partial \Delta} \right. \\
&\quad \times \left(\frac{f_{s4}}{U^f} + \beta f_{s5} \right) + 2(\bar{u}^2 - \bar{v}^2)^2 \\
&\quad \times \left(\frac{1}{U^f} \frac{\partial f_{s4}}{\partial \Delta} + \beta \frac{\partial f_{s5}}{\partial \Delta} \right) \Big] = \bar{\Delta} c\tilde{or}_{sf},
\end{aligned}$$

where

$$\begin{aligned}
c\tilde{or}_{sf} &= -t^{sf2} z \left[\frac{2}{E^2} \left(1 - \frac{\bar{\Delta}^2}{E^2} \right) \right. \\
&\quad \times \left(\frac{f_{s1}}{U^f - 2\bar{E}} + 2 \frac{f_{s2}}{E} - \frac{f_{s3}}{U^f + 2\bar{E}} \right)
\end{aligned}$$

$$\begin{aligned}
&+ \frac{\Delta}{E^2} \left(\frac{1}{U^f - 2\bar{E}} \frac{\partial f_{s1}}{\partial \Delta} + 2 \frac{1}{E} \frac{\partial f_{s2}}{\partial \Delta} - \frac{1}{U^f + 2\bar{E}} \frac{\partial f_{s3}}{\partial \Delta} \right. \\
&+ f_{s1} \frac{\partial}{\partial \Delta} \frac{1}{U^f - 2\bar{E}} + 2 f_{s2} \frac{\partial}{\partial \Delta} \frac{1}{E} \\
&\left. - f_{s3} \frac{\partial}{\partial \Delta} \frac{1}{U^f + 2\bar{E}} \right) - 4 \frac{(E^f - \mu + \frac{U^f}{2})^2}{E^4} \\
&\times \left(\frac{f_{s4}}{U^f} + \beta f_{s5} \right) \\
&+ 2 \frac{(\bar{u}^2 - \bar{v}^2)^2}{\Delta} \left(\frac{1}{U^f} \frac{\partial f_{s4}}{\partial \Delta} + \beta \frac{\partial f_{s5}}{\partial \Delta} \right) \Big].
\end{aligned}$$

Putting $E^f = \mu = \frac{De}{2}$ and $\bar{\Delta} = 0$ in $c\tilde{or}_{sf}$ and assuming that $\beta_c U^f \gg 1$ one obtains (4.9)

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